Lecture 14: Molecular analysis 1

Read: BLB 3.3–3.5
HW: BLB 3:21a,c,e&f,25,29,37,49,51,53
Sup 3:1–8

Know:
• molecular & empirical formulas
• formula & molecular weights

“No Score” from Exam 1?? Not a problem—Go see Mike in 210 Whitmore

Need help?? Get help!! TAs in CRC (211 Whitmore) and Supplemental Instruction (SI)—hours on Chem 110 website; Sheets office hours: Mon 12:30-2; Tue 10:30-12 in 324 (or 326 Chem Bldg)

Keep reviewing what we’ve covered previously in class. We will cover the same concepts over & over again in different contexts and build on what was covered previously.

BST #7 Molecular formulas & structure: Feb 19
Important connections!!!

**Avogadro’s number** $(N_A)$: connects molecules (or atoms) to moles; connects *microscopic* properties to *macroscopic* properties (e.g., g, mL) that are experimentally measurable; **review** Lecture 2.

**Conservation of energy**: energy is not created or destroyed, it just changes its form; **review** Lecture 2.

**Conservation of mass**: mass of products = mass of reactants; **balance the reaction!!!**

**Balanced chemical equation**: connects moles (molecules) of reactants with moles (molecules) of products; related to conservation of mass

**Formula weight**: connects mass to moles; connects a property that can be measured (determined) **experimentally** to moles (or molecules) of substance given in the balanced reaction

**Empirical formula**: tells *relative* number of atoms in a molecule; obtained from %mass or molecular formula
A word about coefficients & subscripts

5 $C_6H_{12}O_6$ molecules of $C_6H_{12}O_6$

atoms of C in $C_6H_{12}O_6$

• Changing coefficient changes the amount of that molecule, not the identity. This is what you change for balancing chemical equations.

• Changing the subscripts changes the identity of the molecule. NEVER, EVER do this to balance a chemical equation!
Formula & molecular weight

• **formula weight (FW):** sum of all atomic weights (in amu) in chemical formula

• **molar mass:** mass of 1 mol; in (g/mol); always numerically equal to formula weight (amu); use it to convert between moles & grams!—talked about this briefly in Lecture 2; please review

\[ \text{C}_6\text{H}_{12}\text{O}_6 \text{ (glucose)} \]

- C:
- H:
- O:

\[ \text{FW} = \text{g/mol} \]

*If compound is a molecule:* FW = molecular weight (MW)

<table>
<thead>
<tr>
<th></th>
<th>FW</th>
<th>MW</th>
</tr>
</thead>
<tbody>
<tr>
<td>C atom</td>
<td>✓</td>
<td>—</td>
</tr>
<tr>
<td>NaCl</td>
<td>✓</td>
<td>—</td>
</tr>
<tr>
<td>C\textsubscript{6}H\textsubscript{12}O\textsubscript{6}</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

• can calculate *percent composition* (% mass contributed by each element) from FW
Example:
How many molecules are present in the US recommended daily allowance for vitamin C (C$_6$H$_8$O$_6$), which is 60.0 mg? How many oxygen atoms are present?
Percent composition

What is the mass percent of C in C\(_6\)H\(_{12}\)O\(_6\)?

FW of C\(_6\)H\(_{12}\)O\(_6\): 180 g/mol

\[
\text{%C} = \frac{\text{mass of element}}{\text{MW of sample}} \times 100
\]

If % C in an unknown substance is 54.2%, a 100 g sample of that substance contains 54.2 g of C.

What if I have 2 g of that sample? How many grams of C are in the sample if it is 54.2% C by mass?
Empirical formula

• *relative* numbers of atoms of each element

• *whole numbers*!!

• *simplest* formula; experimentally determined by obtaining *relative* masses

percent composition ⇒ empirical formula

*Example:*
A compound is made up of C, H & O. Compositional analysis yields the following weight percents. What is the empirical formula?
40.0% C ⇒

6.7% H ⇒

53.3% O ⇒
Molecular formula

- need the **molecular weight** & the **empirical formula**

- **whole numbers!!**

How can we experimentally determine the molecular weight? One way is to use mass spectrometry.

image source: http://antoine.frostburg.edu/chem/senese/101/atoms/slides/sld017.htm
Previous empirical formula example (p 7), con’t.

What is the molecular formula if molar mass is 90.0 g/mol?

*Empirical formula:* CH$_2$O

*Molecular weight of CH$_2$O:*
**Example:**
What is the molecular formula and molar mass of tyrosine, shown below? And btw, what functional groups are present, if any?
Combustion analysis example:

6.52 g of a compound containing C, H and O is completely combusted to yield 9.56 g CO₂ and 3.91 g H₂O. What is the empirical formula of the compound?

*MW of CO₂: 44 g/mol  MW of H₂O: 18 g/mol*
Example:
A petroleum chemist isolated a component of gasoline and found that the molar mass of this hydrocarbon is 114 g/mol. When a 1.55 g sample of this compound is burned in excess oxygen, 2.21 g of H₂O and 4.80 g of CO₂ were produced. Find the empirical and molecular formulas.
Before next class:

Read: BLB 3.3–3.5; 9.1–9.2
HW: BLB 3:21a,c,e&f,25,29,37,49,51,53
     Sup 3:1–8

Know:
• molecular & empirical formulas
• formula & molecular weights
• VSEPR

Answers:
p. 4: 180 g/mol
p. 5: \(2.05 \times 10^{20}\) molecules; \(1.23 \times 10^{21}\) atoms O
p. 6: (top) 40.0% C; (bottom) 1.08 g C
p. 7: CH₂O
p. 9: C₃H₆O₃
p. 10: C₉H₁₁NO₃; 181 g/mol; amine, carboxylic acid, alcohol
p. 11: CH₂O
p. 12: empirical formula, C₄H₉; molecular formula, C₈H₁₈